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ANALYTICAL CHEMISTRY OF 2, 4, 6-TRINITROTOLUENE

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OCTOBER 1980



**US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
LARGE CALIBER
WEAPON SYSTEMS LABORATORY
DOVER, NEW JERSEY**

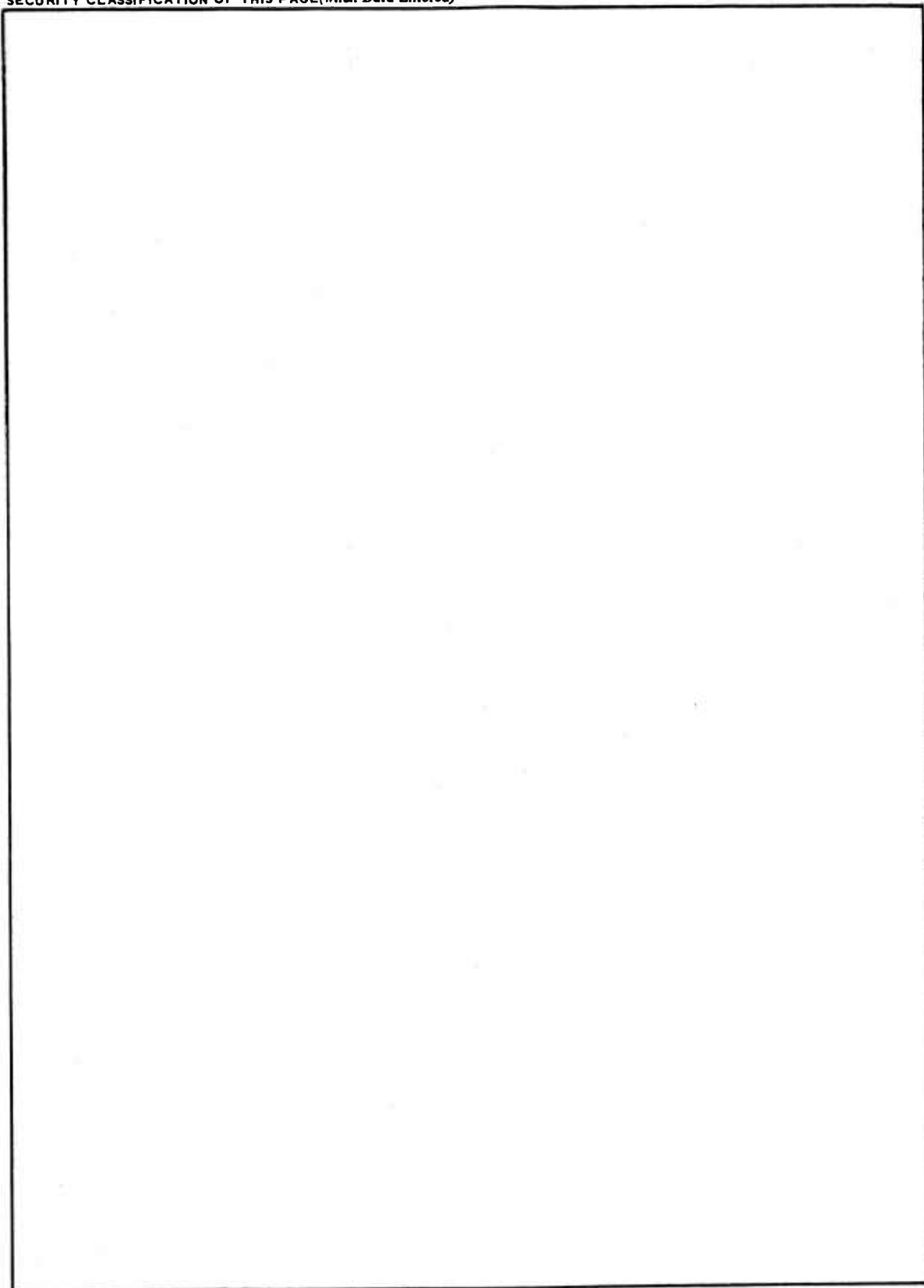
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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER SPECIAL PUBLICATION ARLCD-SP-80007	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) ANALYTICAL CHEMISTRY OF 2,4,6-TRINITROTOLUENE		5. TYPE OF REPORT & PERIOD COVERED Final
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Thomas C. Castorina		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS ARRADCOM, LCWSL Energetic Materials Division (DRDAR-LCE) Dover, NJ 07801		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS ARRADCOM, TSD Scientific & Technical Info Div (DRDAR-TSS) Dover, NJ 07801		12. REPORT DATE OCTOBER 1980
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		13. NUMBER OF PAGES 35
		15. SECURITY CLASS. (of this report) Unclassified
15a. DECLASSIFICATION/DOWNGRADING SCHEDULE		
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release, distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Secondary explosive Spectrophotometry and thermogravimetry Instrumental analysis Electrochemistry Wet chemical analyses Chromatography Spectrometry		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) An annotated bibliography of the analytical chemistry of 2,4,6-trinitro- toluene is presented covering a period from 1940 to 1979, in the areas of wet chemical, thermogravimetric, electrochemical, chromatographic, spectrophotometric, and spectrometric methods of analyses.		

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INTRODUCTION

This annotated bibliography of the analytical chemistry of 2,4,6-trinitrotoluene, alternately referred to as α -TNT or TNT, covers a period ranging from ca. 1940 to the present. Over this period, the field of analytical chemistry and, therefore, that of TNT has advanced from simple wet chemical to automated, computerized, and highly complex instrumental methods. Because of this wide spectrum of advancements, the analytical chemistry of TNT will be formatted according to the general categories of:

- Wet chemical methods
- Thermogravimetry
- Electrochemistry
- Chromatography
- Spectrophotometry
- Spectrometry

Strict adherence to such a format is not possible. The electrochemistry to spectrometry categories are predominantly instrumental. However, although wet chemistry predates these categories, it nevertheless pervades the most sophisticated instrumental technique to date. In addition, in some cases one of the disciplines within a category will be interfaced with one of another category, e.g., mass spectrometry/gas chromatography (GC/MS). In such cases the referenced analyses will be cited under one category and cross-referenced under the other.

Wet Chemical Methods

The qualitative analysis of explosive mixtures containing TNT entails laborious and time consuming procedures predicated on specific knowledge of solubilities, melting points, densities, and refractive indices. Procedures for the determination of these constants (ref 1) together with some qualitative and quantitative spot test methods are compiled in a series of manuals (ref 2). Military specifications of the physical constants for TNT are also delineated (ref 3), and those of TNT in various formulations, amatol, octol, tetrytol, pentolite, tritonal, Comp. B, Comp. B-3, Comp. B-4, Comp. C-3, Comp. C-4, cyclotol, DBX, ednatol, HBX-3, H-6, HTA-3, minol, and MOX-2B, are tabulated in an engineering design handbook (ref 4).

Wet chemical methods of analyses of formulations containing TNT, as cited above, usually involve the application of preferential dissolution for resolving the mixture into its component parts (ref 5). Titrimetric methods for the quantitative determination of the resolved components are also presented (refs 6, 7, 8, 9, 10).

Specific problem solving and modifications of procedures by wet chemical methods are included as recorded in the Picatinny Arsenal Laboratory Reports (PALR). Acidity values as sulfuric acid were found to be comparable with various indicators (ref 11). The determination of percent TNT in tetrytol by a carbon tetrachloride extraction method was shown to have an accuracy and reproducibility of $\pm 0.03\%$ and 0.04% , respectively (ref 12). A mixture consisting of TNT, Haleite (EDNA), and cyclonite (RDX) was analyzed by extractions, $\text{CHCl}_3/\text{CCl}_4$ for TNT, $3\% \text{NH}_4\text{OH}$ for Haleite and the residue cyclonite by difference (ref 13). Feigl's spot test method was used for the detection of mercury contamination in TNT (ref 14). A mixture of TNT, pentaerythritol tetranitrate (PETN), and wax was analyzed by solvent extractions followed by titrimetry using titanous sulfate (ref 15). The setting point of TNT determined by the inclusion of calcium chloride was found superior, requiring less time than the specification method (ref 16). A modified Fischer method as compared to the specification method was shown to quantify the water content more accurately (ref 17). The compositional analysis of a cast mixture of TNT/RDX/wax/barium stearate was performed by solvent extractions followed by gravimetry (ref 18). A titanous reduction method for the quantitative determination of TNT has been reported (ref 19) and a nonaqueous titrimetric method applied to a mixture consisting of TNT, NH_4NO_3 and NaNO_3 (ref 20).

Results are presented of various spot tests on a select number of ions and organic compounds (including TNT) extracted from explosion debris (ref 21). Single component distributions in cast binary systems with a common TNT matrix were determined by a staining method (ref 22). Development of a detection spray reagent system for the detection of explosive residues (TNT) on the exterior of letter and package bombs is reported (ref 23). A spot test was used for TNT contamination in a powder containing NC, dinitrotoluene (DNT), and dibutyl phthalate (DBP) (ref 24). A detailed review of color reactions and related analytical procedures for the qualitative determination of TNT and formulations containing TNT is given in reference 25. A compilation of analytical data on the more common explosives (TNT) dealing with some color reactions are also compiled (refs 26, 27).

Total nitrogen of TNT in wastewater was determined by preliminary digestion with $\text{K}_2\text{S}_2\text{O}_3$ in alkaline solution and the NO_3 released was reduced by an automated Cd reduction method (ref 28). Trinitrobenzoic acid was dissolved in water and titrated with NaOH without an indicator until a weak pink color appeared and persisted even in the presence of TNT and trinitrobenzene (TNB) (ref 29). A gas comparison pycnometer used in conjunction with a Velidyne D15 differential pressure transducer with HE yields a density accuracy of

± 0.002 g/mL (ref 30). The use of acetone as a solvent for 2,4,5-trinitrotoluene caused hydrolysis of the 5-nitro group on standing. The effect is discussed in terms of the sampling factors involved and their importance in trace analysis in general (ref 31). The chemical analysis of TNT by extraction and titration techniques, as well as by gas chromatography (GC), is reported (ref 32). Simple chemical and instrumental procedures are given for the identification of common explosives (TNT included) in post-explosions (ref 33). Titrimetry and ultraviolet (UV) analyses were used to quantify components of a mixture resolved by column chromatography (ref 34). After treatment of wastewater samples containing TNT and its derivatives with sodium sulfite-hydroxide, quantitative determinations were made using a spectrophotometric procedure (ref 35).

Thermal Analysis

Differential scanning calorimetric (DSC) methods are applied for the determination of heat of fusion, purity, specific heat, and activation energy of decomposition for undiluted, unmixed samples of TNT, TNB, tetryl, RDX, HMX, and PETN (ref 36). The differential thermal analysis thermograms of TNT showing varying rapidity of heat feedback is assumed to be the cause of differing exotherms observed with mixtures of TNT and carborundum (ref 37). Observations with DSC indicate polymorphic or polytypic behavior near the melting point of TNT (ref 38). The thermal properties of TNT have also been reported by Maycock (ref 39). Calorimetric and X-ray data show that structural changes can occur in TNT on heating and that different forms can be prepared by crystallization and sublimation (ref 40). A review is presented with emphasis on hot-stage microscopy studies of pour points of casting of TNT into artillery rounds (ref 41). Hot-stage microscopy technique was used to determine the wettability of the TNT/RDX in Comp. B by wax after solidification of TNT (ref 42).

Electrochemistry

Trinitrotoluene was determined in the presence of DNT's by polarography in a medium containing Me_2CO , pH buffer, and Na_2SO_3 (ref 43). A review with 15 references on the polarographic behavior of 20 explosives and further developments in the field are reported (ref 44). Applicable to both lab and field use, the single sweep polarographic technique can determine as little as 50 ppb directly from water medium (ref 45). Pulse polarography was applied for the qualitative and quantitative analysis of trinitroglycerine in TNT (ref 46). Polarographic analysis of some explosives including TNT have been documented (ref 47). A review of the state of development of the various instrumental methods of analyses including polarography is presented (ref 48). Whitnack (refs 49, 50) also used

the linear sweep polarograph to determine microgram quantities of TNT in milligram samples of warhead exudates. Brandone, et al. (ref 51) determined polarographically the composition of explosive mixtures containing TNT.

The acid/base behavior of aromatic nitro compounds in dimethyl formamide (DMF), Me_2CO , MeCOEt , and a mixture of solvents were studied using high frequency titration (ref 52). $\text{Pr}_2\text{CO/EtOH}$, MeEtCO/EtOH are reported as suitable solvents for the potentiometric titration of TNT (ref 53). Low concentrations of TNT in air were detected in their negatively charged state via electron transfer from ionized SF_6 . The charged TNT was measured with an air electron multiplier producing an electric current proportional to its concentration (ref 54).

Chromatography

Gas Chromatography

Explosive detection is enhanced by preconcentration on a metal surface of available explosive vapor prior to its introduction into the GC detector. Adsorption by a metal surface has the additional advantage of reduced water interference, easier thermal cycling, reduced memory effects, and greater durability (ref 55). A quantitative GC procedure was developed to measure the output of vapor concentrations of TNT, 2,4-DNT and EGDN (ref 56). Vapors of TNT were concentrated on chromosorb 102 at 50°C - 70°C and detected by GC (ref 57). Experimental techniques were employed involving measurement of response of test equipment to a controlled flow of TNT vapor source and determinations made of the vapor concentration by trace GC equipped with a vapor concentrator (ref 58).

Gas chromatography, in conjunction with thin layer chromatography (TLC), was used for the quantitative analysis of nitro aromatic compounds (TNT) in the micro- to pico-gram range using Ni-63 electron capture detector (refs 59, 60). Hoffsommer also developed a GC method for the detection of TNT together with RDX and tetryl in ppb to pp trillion in sea water (refs 61, 62). Isomer impurities of MNT, DNT, and TNT in alpha-TNT were resolved and quantified by GC (refs 63, 64, 65, 66, 67, 68). A GC procedure using a flame ionization detector was developed to control product quality and study variables in the continuous TNT process (ref 69). Products of biodegradation of TNT in a matrix of TNT were analyzed by GC using a glass column packed with Dexsil 300 on chromosorb W. (ref 70). After an explosion, the base charge residue containing TNT extracted with acetone from a blasting cap was determined by GC with a Ni-63 electron capture detector (ref 71). A mixture of TNT and 1,3-

dinitrobenzene was resolved and quantified by GC (ref 72). The GC analysis of TNT in mixtures was compared to chemical analysis by extraction/titration techniques (ref 32). Sampling factors involving GC trace analysis of TNT is discussed in terms of chemical instability in acetone (ref 31).

A number of domestic and foreign military TNT samples were analyzed by the GC headspace pressure of TNT and the partial pressures of several associated impurities (ref 73). The GC headspace pressure technique was also shown to preclude the necessity for ultrapure sample and with the electron capture detector to be sensitive to 10^{-7} torr and experimentally simple (ref 74). The vapor pressures of TNT and DNT isomers were measured by the GC electron capture technique (ref 75).

Gas chromatography indicated that 2,4,6-trinitrophenol and 3,5-dinitrophenol are formed predominantly from TNT with NaOH (ref 76). The colorimetric method as compared to GC required less work, gave a position response for all TNT isomers, including degradation compounds, and was more suitable for routine surveillance (ref 77). The GC chromatograms are compiled together with TLC data and color reactions of TNT and TNT in mixtures (ref 26). A review is presented of the state of development of the gas chromatographic technique for the analysis of explosives, TNT included (ref 48). Prototypes of on-stream process analyzers have been developed utilizing the latest technological advances in physicochemical sensors and instrumentation (GC) for the detection and measurement of the process control parameters in the manufacture of TNT (ref 78). The more advanced instrumental methods of analysis, including GC, for the detection and identification of explosives are presented (ref 79).

Pyrolysis of explosives in tandem with GC/MS was used for the identification of contaminant explosives in the environment (ref 80). Isomer vapor impurities of TNT were characterized by GC-electron capture detector and mass spectrometry (ref 81). Volatile impurities in TNT and Comp. B were analyzed using a GC/MS; the GC was equipped with electron capture and flame ionization (FI) detectors (ref 82). The vapors evolved from mines, TNT, acetone, toluene, cyclohexanone, and an organosilicon, were analyzed by GC/MS (ref 83). Red water produced by the sellite purification of crude TNT was analyzed by GC/MS for potentially useful organic compounds, 2,4-dinitrotoluene, 3- and 4-sulfonic acids (ref 84). Various reports were surveyed to determine which methods, including GC/MS, are potential candidates for detection of traces of TNT vapors emitted from land mines; factors influencing transportability of TNT vapors through soil to soil/air interface are discussed (ref 85). Impurities contained in TNT were analyzed by a GC equipped with a FI

detector and interfaced with a MS; spectra were recorded on photoplates and processed by a computer system (ref 86). A GC method was studied for the detection and identification of post-explosion gas phase residues (ref 87). Gas chromatography was used to support work on enzymatic action on TNT to produce photons at 492 nm detected photometrically at the pp trillion level (ref 88). Wastewaters from the Army manufacture of TNT were characterized by GC/TLC and found to contain more than 40 organic compounds derived from TNT and its isomers (ref 89). Gas chromatography, in combination with TLC and spectroscopic methods, has been reported (ref 90) for the identification of post-explosion residues.

Thin Layer Chromatography

Two dimensional TLC was used to identify impurities derived from TNT in Comp. B (ref 91). Micro quantities of TNT impurity in DNT were determined with fine-grained (2.5-10 μ) silica gel on microplates (ref 92). The TLC separations of all major impurities formed during the purification step (ref 93), and from various steps of the continuous TNT process are reported (ref 94). Development of thin-layer chromatograms of impurities in TNT was achieved by direct incorporation of a zinc reductor in the thin-layer material (ref 95). Organic explosive residues, e.g., TNT, were detected by TLC utilizing a combination of R_f values and color development (ref 96). High explosives having the same R_f values on thin-layer chromatograms and difficult to separate were readily resolved as their colored complexes with aromatic amines (ref 97). The identity of 21 compounds, including nitrotoluenes, was achieved by TLC using 6 solvents with 4 spray reagents (ref 98). Traces of TNT and other explosives adhering to surrounding objects after an explosion can be detected and identified by TLC in combination with initial UV, followed by chemical visualization (ref 99). A quantitative method of analysis of polynitroaromatics (TNT and its isomers included) in complex mixtures by combination of TLC with visible spectrophotometry is described (ref 100). A short column containing porous polymer beads was used to collect explosive vapors of TNT, followed by TLC analysis of post-explosion debris (ref 101).

A TLC/GC procedure was developed for determining TNT and other explosives in ocean floor sediment (ref 60). A TLC method is employed for the detection and identification of post-explosion solid residues (refs 42, 90). Thin layer chromatography was used together with GC and high performance liquid chromatography (HPLC) to support work on enzymatic action on TNT (ref 88). Wastewaters from Army manufacture of TNT were characterized by TLC/GC (ref 89). The more advanced aspects of TLC, such as high performance 5 micron size, C18 silica gel with UV-fluorescence indicator, was used for the detection

of explosive residues (ref 79). Data on TLC and color reactions of TNT in mixtures are furnished (ref 7). Purification by-products in the manufacture of TNT by the continuous process were identified by TLC in conjunction with infrared (IR) and nuclear magnetic resonance (NMR) (ref 102).

High Performance Liquid Chromatography

The analysis of TNT in wastewaters is made simple and direct by liquid chromatography (LC) using a UV detector at 220 nm (refs 103, 104). A LC method suitable for the low level determination of tetryl in the presence of TNT, RDX, and HMX is described (ref 105). The adsorptive LC of TNT was demonstrated using poly (styrene-divinyl benzene) adsorbent and ethanol as the moving phase (ref 106). A HPLC was used for the separation of TNT from purification by-products of hexanitrobibenzyl (ref 102). Enzymatic action on TNT was supported by HPLC (ref 88). The HPLC chromatograms of TNT are included, together with data on TLC and color reactions of TNT in mixtures (ref 26). Pollutants in wastewater effluents containing TNT were resolved by HPLC and quantified (ref 107). Micrograms 30-40, of resolved fractions by HPLC were concentrated onto 6 mg of KBr and examined by IR (ref 108). The HPLC and the chemical ionization mass spectrometry (CIMS) were used in the isolation and identification of explosive residues (ref 109).

Column Chromatography

Components of an explosive mixture containing TNT were resolved by column chromatography and quantified by titrimetric and UV analyses (ref 34). The mixture of products of thermal decomposition of TNT were resolved by column chromatography (ref 110).

Spectrophotometry

Ultraviolet Spectrophotometry

A spectrophotometric analysis is described of water effluent from carbon columns processing pink water on a continuous real-time basis down to 0.1 ppm of TNT (ref 111). The TNM impurity in TNT was determined spectrophotometrically at a sensitivity level of 0.005% (ref 112). The spectra of 1:1 charge-transfer complexes of diamines with TNT were generated and methods developed for determining TNT in the presence of hexogen, octagen, and waxes (ref 113). A spectrophotometric procedure for the quantitative analysis of TNT in derivatives of TNT after sulfite-hydroxide treatment of wastewater samples is reported (ref 35). An UV analysis was used for the

detection and quantitative determination of TNT in a formulation (ref 34). Ultraviolet spectroscopy was employed for the identification of post-explosion residues including TNT (ref 90). With increasing NaOH concentration, the absorption maximum of TNT exhibits a bathochromic shift (ref 76). A prototype of on-stream UV analyzer in real time is described (ref 78). A review of the state-of-development of instrumental methods including spectroscopic procedures is presented (ref 112). The UV, together with spectrometric methods, were applied for the characterization of TNT interaction with the surface of carbon (ref 114). A fluorescent-dyed quarternary ammonium ion exchange resin was irradiated with UV light and the fluorescent output was monitored by a photomultiplier. In this manner, TNT was detected in wastewater at the 70 ppb level (refs 115, 116). A literature review was conducted of aspects of bioluminescence pertinent to explosive detection, including TNT, via vapor interaction with microbiological specimens (ref 117). A biochemical approach was used to detect TNT based on two sequential chemical reactions catalyzed by specific ions producing photons read by a photomultiplier tube (ref 118).

Trinitrotoluene vapor in air was determined by a colorimetric method involving a sodium sulfite-hydroxide color complex (ref 119). A method is presented for the quantitative spectrophotometric analysis of polynitroaromatics as the IR "Meisenheimer" complexes in ethylenediamine dimethylsulfoxide solutions (ref 120). Detection by formation of colored reaction complexes determined by wavelength absorbances and absorptivities of the reagent/explosive samples are described (refs 121, 23). A semi-quantitative colorimetric determination is reported of TNT in the presence of TNT and DNT isomers, and checked by GC analysis for the indirect estimation of the total isomer content in the crude TNT (ref 122). A colorimetric dual channel system was used to measure TNT among other explosives in wastewater effluents at army ammunition plants (AAP's); the determination of TNT is reported to be sensitive to the 1 ppm level (ref 123). The colorimetric method, as compared to GC, required less work, gave a position response for all TNT isomers, including degradation products, and was more suitable for routine surveillance (ref 77).

Infrared Spectrophotometry

Constituents, including TNT in various compositions, were detected and identified rapidly using IR (ref 124). An IR method was developed for the estimation of α , β , γ -TNT and 2,4-DNT (ref 125). A compilation of IR spectra is presented of ingredients of propellants and explosives; the IR spectra of the various isomers of TNT are included (ref 126). The isomers of MNT, DNT, as well as TNT,

determined by IR have also been reported (refs 127, 128, 129). Four explosives, including TNT and an explosive mixture containing TNT, were discriminated on the basis of the sapphire cell spectra alone (ref 130). The presence of TNT/RDX was established in the exudates from munitions by IR and Raman spectroscopy (ref 131). Microgram quantities of HPLC-resolved fractions containing TNT were examined by IR as micro-pellets using a beam condenser (ref 108). The IR spectra of US military and foreign samples of TNT are presented (ref 79). The IR was used for the identification of explosive residues (TNT, RDX, PETN) detected at the scene of criminal bombings (refs 90, 132). The identification of purification by-products in the manufacture of TNT was achieved by IR, together with TLC, and NMR techniques (ref 102). Infrared spectra of TNT are included in the compilation of other spectrograms and chromatograms (ref 26). The IR, in conjunction with MS and electron spectroscopy (ESCA), was applied for the study of the interaction of TNT with the surface of carbon (ref 114). A review is presented of the state-of-development of instrumental methods, including IR, for the analysis of TNT (ref 48).

Spectrometry

Nuclear Magnetic Resonance

Radio frequency resonance absorption spectroscopy techniques involving NMR, electron spin resonance, and nuclear quadrupole resonance (NQR), were investigated for the detection of specific explosives, e.g., TNT hidden in airline luggage (ref 133). An NMR procedure was developed for determining low concentrations (0.1% to 1%) of unsymmetrical TNT isomers in crude and refined TNT (ref 134). Nonvolatile impurities in crude and refined TNT were characterized by NMR (ref 135). The NQR was used for the determination of the chemical structure, crystalline states, and morphology of TNT (ref 136). The NMR was used, together with IR and TLC, for the identification of the purification by-products in the manufacture of TNT (ref 102). The NMR spectra of TNT are in the compilation of other spectral and chromatographic data of the more common explosives (ref 26). A review is presented of the state-of-development of instrumental methods, including NMR, for the analysis of TNT (ref 48).

X-Ray Spectroscopy

X-ray and calorimetric data show that structural changes can occur in TNT on heating and that different forms can be prepared by crystallization and sublimation (ref 38). Differences in the X-ray diffraction patterns of TNT were shown to be based on the method of

preparation of 1 TNT (ref 37). Post-explosion debris were examined by a Gandolfi camera, requiring but a single crystal of TNT of micron size for identification purposes (ref 137). The X-ray diffraction patterns of TNT are included, together with those of hexanitrostilbene (ref 138).

Mass Spectrometry

An extensive and detailed coverage of the MS of explosives in general has been documented (ref 139). Volatile constituents of Comp. A-3, Comp. B, pressed TNT, and cast TNT were surveyed with a residual gas analyzer MS (ref 140). The mass spectra of all possible TNT (except for 3,4,5-TNT) and DNT isomers in the vapor phase were obtained as a function of ionizing voltage (refs 141, 142). The use of membrane inlet systems for the separation of TNT vapor in trace vapor detection is described and an analysis of the membrane inlet system for quadrupole mass spectroscopy is presented (refs 143, 144). Estimations of the vapor pressure of TNT were made mass spectrometrically in the range of 50°C-143°C by the Knudsen method, making possible the determination of concentrations of TNT in air as a contaminant (ref 145). The use of MS for the in situ detection of TNT in air was studied; the lower limit of detection is reported to be 5×10^{-14} volume parts of TNT (ref 146). Trace elemental impurity profiles of TNT from various AAP's were related to their source of origin using a double focusing spark source MS, complemented with atomic absorption spectrometry (refs 147, 79). Mass spectrometry, together with electron spectroscopy (ESCA), was used for the characterization of TNT interaction with the surface of carbon (ref 114). A review of the mass spectrometric techniques for the analysis of explosives is presented by Yinon (ref 48). The MS spectra of TNT are included in the compilation of other spectral and chromatographic data of the more common explosives (ref 26). In addition, the mass spectra of TNT have been reported by other investigators (refs 148, 149, 150).

Mass Spectrometry Interface with Gas Chromatography

The pyrolysis products of explosives in tandem with GC/MS served as indirect identification of contaminant explosives in the environment. The pyrolysis products generated, which are indicative of the parent molecule, are separated by GC and identified by MS (ref 80). Red water produced by the sellite purification of crude TNT was analyzed by GC/MS for potentially useful organic compounds, 2,4-DNT, 3- and 5-sulfonic acids (ref 84). The enhanced detection of TNT vapors was achieved by pre-concentration on a metal surface, and flash-desorbed onto a chromatograph interfaced with a quadrupole MS

(ref 55). Vapors of TNT, acetone, toluene, cyclohexanone, and an organosilicon were detected and identified by GC/MS (ref 83). Various reports were surveyed to determine which methods, including GC/MS, are potential candidates for the detection of traces of TNT emitted from military land-mines (ref 85). The vapors collected from Comp. B were analyzed by GC/MS; besides the TNT and RDX, H_2O , N_2O , CO_2 , plus several unidentified compounds, were detected (ref 82). By the use of GC, isomeric impurities in the vapor, as well as solid phase of TNT, were resolved and identified by MS (refs 81, 86, 151).

Negative-Ion Mass Spectrometry

The detection of TNT in trace vapor quantities was demonstrated by negative-ion mass spectrometry (NIMS) to be sensitive (1 ppm) and selective (refs 152, 153). The TNT was analyzed using an electron probe to produce a negative charge on TNT, followed by quadrupole MS with SF_6 as a diluent (ref 154).

Plasma Chromatography Mass Spectrometry

Due to the extremely electronegative character of nitroaromatics, e.g., TNT and its isomers, and their large cross section to charge-transfer and ion-molecule reactions, negative ion plasma chromatography MS has been found particularly suitable for their detection and identification (ref 155). The TNT was detected in air at 10 pp trillion (mol/mol) with plasma chromatography mass spectrometry (PCMS) as a function of carrier gas flow (refs 156, 157). The detection of TNT vapors with an ion mobility spectrometer, a type of PCMS, is described, together with other methods of detection (ref 158). The detection of TNT vapors by PCMS and EIMS have been evaluated and found to be limited by the lack of portability of TNT vapors through barrier materials (ref 159). The PCMS was found to be ideally suited for explosive vapor detection, operating at atmospheric pressure, and responding to nitrated compounds such as TNT and DNT (ref 160).

Chemical Ionization Mass Spectrometry

A CIMS was used for the detection of TNT/DNT vapors in ambient air with a detectability limit of 0.06 nanogram/ M^3 (ref 146). The CIMS was used for the identification of explosives as a function of reagent gases; TNT was identified by CIMS in a post-explosion residue (ref 161). The chemical ionization/electron impact (CI/EI) spectra of 10 derivatives of TNT have been reported (ref 162). The use of methane as a reagent gas generates a CI mass spectrum of TNT with a predominant M^{+1} ion which facilitates identification (ref 163). The CIMS of TNT with hydrogen as reagent gas produces ions of low

abundance from the ensuing ion-molecule reactions and, as such, confirm molecular weights (ref 164). The CIMS fragmentation patterns of civilian and military explosives were shown to be sensitive to source temperature and pressure of reagent gas (ref 165). The NH_3 reagent gas was used for the CIMS identification of explosive residues (ref 109). Components of technical grade mixtures of explosives were identified by field desorption MS via their intense molecular ions or protonated molecules and structurally significant fragmentations (ref 166). Concentrations in air of various explosives, including TNT, were measured by means of isotope dilution using field ionization mass spectrometry to measure the relative abundance ratios (ref 167).

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